Coexistence of superfluid and Mott phases of lattice bosons

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Recent experiments on strongly-interacting bosons in optical lattices have revealed the coexistence of spatially-separated Mott-insulating and number-fluctuating phases. The description of this inhomogeneous situation is the topic of this Letter. We establish that the number-fluctuating phase forms a superfluid trapped between the Mott-insulating regions and derive the associated collective mode structure. We discuss the interlayer's crossover between two- and three-dimensional behavior as a function of the lattice parameters and estimate the critical temperatures for the transition of the superfluid phase to a normal phase.

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Dilute gases of ultra-cold bosons on a lattice present a model system for exploring quantum phases of matter. Experiments in optical lattice traps have demonstrated controlled tunability through a quantum phase transition between a Mott-insulating phase which has fixed particle number on each lattice site and a phase exhibiting number fluctuations [1, 2]. As has been recently observed in radially symmetric traps [3, 4], for sufficiently deep optical lattice potentials the system arranges itself into a "wedding cake structure" in which Mott-insulating phases of bosons commensurate with the lattice alternate with interlayers of incommensurate bosons with fluctuating site occupancy [5, 6, 7, 8]. Various questions concerning such inhomogeneous systems have so far been unanswered in both theory and experiment: is the interlayer associated with number fluctuations a condensate? If so, in what temperature range is the condensate robust? Is there collective behavior in the interlayer, analogous to that seen in bulk superfluids? How does the system crossover from three-dimensional to two-dimensional behavior as the interlayer thickness is varied? Understanding these issues would also be important for related avenues in cold atomic physics, such as the interplay of spatial inhomogeneity and quantum criticality [9], realization of robust states for quantum computation [10], and the physics of interacting fermions on a lattice [11].

It has been established that dilute gases of bosons in optical lattice potentials are well-described by the Bose-Hubbard Hamiltonian [5, 12] in which the bosons' movement between sites is characterized by a tunneling term $\mathcal{H}_J = -J\sum_{\langle ij\rangle} a_i^\dagger a_j$ related to the overlap of the single-particle wave functions between neighboring sites i and j, and the on-site interaction is modeled by $\mathcal{H}_U = (U/2)\sum_i n_i(n_i-1)$. It is the external trapping potential, $V(\mathbf{r}_i)$, which is responsible for breaking the uniformity of the system and promoting spatial coexistence of the Mott insulating and superfluid phases at large interaction [5, 6, 7, 8]. Analytical treatments of the inhomogeneous system are complicated by the fact that no simple approximation of the Hamiltonian can faithfully describe the entire phase space. The Bogoliubov approximation [13, 14] captures the condensed phase for large J/U but breaks down close to the Mott regions. The decoupled-site approximation [9, 13, 15, 16], valid when $J \ll U$ and the boson density is close to a commensurate value, works well within and close to the Mott regions but fails deep within the incommensurate phase. A third possibility is presented by the "pseudo-spin" approximations [17, 18, 19], valid for intermediate values of J/U, which bypass these shortcomings by treating kinetic energy and interactions on comparable footing.

In this Letter, we employ a pseudo-spin approximation of the Bose-Hubbard model to describe the inhomogeneous systems where the density of bosons varies as a result of a confining trap. Concentrating on a single interlayer trapped between two Mott-insulating phases, we show that number fluctuations give rise to a condensate with a well-defined order parameter and derive the dynamical equations governing the system. We obtain the collective excitation spectrum of the interlayer condensate and show that in the homogeneous limit, it properly reproduces the known properties of bulk superfluids. We explore the behavior of the collective modes as a function of the thickness of the interlayer and show that they provide a signature of dimensional cross-over in the condensate, which can be achieved by tuning experimental parameters. We conclude with a brief discussion of the expected mean-field critical temperature T_c of an interlayer superfluid and its behavior as a function of interlayer thickness.

Focusing our attention on the Mott phases with integer boson filling n and $n+1$ and the superfluid phase at intermediate fillings, we consider a Hilbert space restricted to the number-basis states $|n\rangle$ and $|n+1\rangle$ at each site. Considering the excluded states $|n-1\rangle$, and $|n+2\rangle$, we find that their contribution to the energy is of order of J^2/U. We note that the number-fluctuations on sites are driven by the incommensurability of bosons with the lattice in the presence of the trapping potential. The truncated Hilbert space in the limit $J/U \ll 1$ may be represented by

the spin-1/2 states [15, 18], $|n+1\rangle = |\uparrow\rangle$ and $|n\rangle = |\downarrow\rangle$, the eigenstates of the operator s^z with eigenvalues $\pm 1/2$. The tunneling term in the Bose-Hubbard Hamiltonian can be identified with raising and lowering spin-1/2 operators, s^+ and s^-, such that $a_i^\dagger a_j \to (n+1)s_i^+ s_j^-$, where $a_i^\dagger$ is the boson creation operator on site i. The interaction and the potential energy terms are diagonal in the number basis at each site and the boson number operator ($\hat{n}_i = a_i^\dagger a_i$) can be expressed in terms of the spin-1/2 matrix s^z, $\hat{n} = n + 1/2 + s^z$. Thus, in the truncated Hilbert space, one obtains an effective Hamiltonian identical to the spin-1/2 XY model in the external "magnetic" field:

$$\mathcal{H} = -J(n+1)\sum_{\langle ij\rangle}\left(s_i^x s_j^x + s_i^y s_j^y\right) + \sum_i (Un - \mu_i)s_i^z. \quad (1)$$

Here, $\langle ij\rangle$ denotes a summation over nearest neighbors sites, and $\mu_i = \mu - V(\mathbf{r}_i)$ defines the chemical potential offset by the external trapping potential, $V(\mathbf{r}_i)$. The chemical potential μ is set by the total number of particles in the system, $\langle N\rangle = \sum_i \langle \hat{n}_i\rangle$.

The pseudospin operators are coupled ferromagnetically in the x-y plane and therefore, at low temperatures can form an ordered state with broken $U(1)$ symmetry in the plane. At the mean-field level, in the ground state configuration, pseudospins are aligned with the local "magnetic" field, $\mathbf{B}_i^0 = zJ(n+1)\,[2\langle s_i^x\rangle, 2\langle s_i^y\rangle, \cos\theta_i]$, where $\cos\theta_i = (\mu_i - Un)/(zJ(n+1))$, and we have assumed $\langle \mathbf{s}_i\rangle \approx \langle \mathbf{s}_j\rangle$ for nearest-neighbors. The equilibrium components of the pseudospin at site i are parameterized by angles on the sphere:

$$\langle s_i^z\rangle = (1/2)\cos\theta_i, \quad \langle s_i^+\rangle = (1/2)\, e^{i\varphi}\sin\theta_i, \quad (2)$$

where the angle φ independent of site index expresses the phase coherence in the system. The continuous degeneracy in the ground state is illustrated in Fig. 1. In the Mott phase, the pseudospins are completely polarized along the z direction, i.e. $\langle s_i^z\rangle = \pm 1/2$, allowing the identification of $\mu_\pm = Un \pm zJ(n+1)$, the values of the chemical potential at the boundaries of the Mott states with n and $n+1$ bosons per site (see Fig. 1). In the xy-symmetry broken phase, $\langle a^\dagger\rangle = \langle s^+\rangle/\sqrt{n+1} \neq 0$ and we have a condensate with order parameter

$$\Delta = (1/N_{\rm inter})\sum_i \langle s_i^+\rangle, \quad (3)$$

where $N_{\rm inter}$ is the number of lattice sites between the two Mott phases.

The locations and sizes of the interlayers can be determined by the relationship $\mu_\pm = \mu - V(\mathbf{r}_\pm)$, where the chemical potential, μ, is obtained self-consistently by fixing the total number of particles in the system, N. For radially-symmetric traps, a simplification occurs in the limit of a thin interlayer, $\delta r_n \ll r_n$ (where r_n is the radius at the center of the interlayer between two

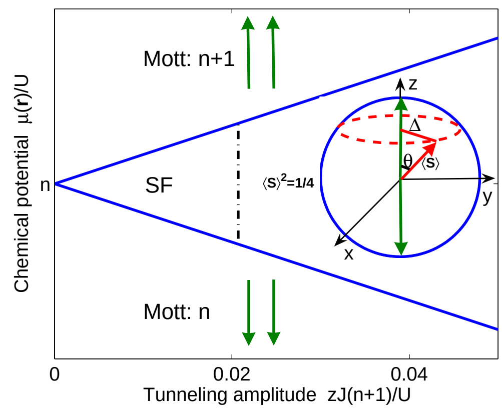

FIG. 1: The mean-field phase diagram for the Bose-Hubbard Hamiltonian. The dash-dotted line corresponds to the interlayer with fluctuating site occupancy. Spontaneous symmetry breaking in the ground state is shown on the sphere $\langle \mathbf{s}\rangle^2 = 1/4$: the equilibrium configuration $\langle \mathbf{s}\rangle$ is degenerate on the circle (dashed line) with nonzero order parameter $|\Delta| = (1/2)\sin\theta$. North and South poles of the sphere correspond to Mott states with $n+1$ and n bosons per site, respectively.

Mott states with particle occupation n and $n+1$ and δr_n is its thickness). In this case, the trapping potential can be linearized around r_n and we find that the number of particles in the interlayer is the same as in the case $J/U = 0$, where the interlayer region would be filled with n and $n+1$ Mott phases. Hence, the chemical potential at small J/U can be found by setting $N = (4\pi/3)\sum_{n=0}^{m-1}(r_n/\ell)^3$, where m is the total number of Mott states in the trap and ℓ is the lattice spacing [8]. We find that for a three-dimensional parabolic trapping potential, $V(r) = \alpha r^2$, the interlayer parameters are given by $r_n = (\mu/\alpha)^{1/2}\,[1 - nU/\mu]^{1/2}$, $\delta r_n = 6J(n+1)/(\alpha r_n)$ when $n > 0$, and $\delta r_0 = 3J/(\alpha r_0)$. These results show that it is possible to tune the width of the interlayers from $\delta r_n \simeq \ell$ to $\delta r_n \gg \ell$, effectively changing the dimensionality of the layers. As a characteristic example in the range of recent experiments [3, 4], a system with trap curvature $\alpha \approx h \times 24\,\mathrm{Hz}/\mu\mathrm{m}^2$, total particle number $N \approx 10^6$, lattice spacing $0.43\,\mu$m, interparticle interaction $U \approx h \times 10\,$kHz and tunneling strength $J \approx h \times 120\,$Hz hosts two Mott regions with $n = 1$ and $n = 2$, and two interlayers. The corresponding interlayer parameters are $r_0 \approx 25\,\mu$m and $\delta r_0 \approx 0.5\,\mu$m; $r_1 \approx 14\,\mu$m and $\delta r_1 \approx 4\,\mu$m. We remark that for a harmonic trap, when gravity is taken into account, the system experiences a shift along the direction of the gravitational field, but is otherwise unaffected.

Having identified the interlayer region, we now turn to the low-energy collective modes within the interlayer. These modes can be calculated using the Heisenberg equations of motion for the pseudospin operators,

$\partial_t \mathbf{s}_i = i[\mathcal{H}, \mathbf{s}_i]$. In the mean-field approximation, one obtains the Bloch equations, $\partial_t \langle \mathbf{s}_i \rangle = \langle \mathbf{s}_i \rangle \times \mathbf{B}_i$, where the effective magnetic field is given by $B_i^+ = J(n+1)\sum_j 2\langle s_j^+ \rangle$ (summation is over the nearest neighbors of site i), and $B_i^z = zJ(n+1)\cos\theta_i$. Assuming that the characteristic wavelength of the excitations is much larger than the lattice spacing ℓ, we approximate the sums entering the effective magnetic field $\mathbf{B}$ by their continuum limit, $\sum_j \langle \mathbf{s}_j \rangle \approx z\langle \mathbf{s} \rangle + \ell^2 \nabla^2 \langle \mathbf{s} \rangle$. The resulting Bloch equations can be analyzed as follows. The equilibrium number density of bosons in the interlayer is $\rho_0 = n + 1/2 + \cos\theta/2$ and the number density $\rho = \rho_0 + \delta\rho$ obeys the continuity equation $\partial_t \rho + \nabla \mathbf{j} = 0$ with the current density $\mathbf{j} = (J(n+1)/2)\sin^2\theta\, \nabla\varphi$. Using the relationship between the canonically conjugate density deviation $\delta\rho$ and the phase, $\partial_t \varphi = -2zJ(n+1)\delta\rho$, one obtains the following differential equation for density fluctuations around equilibrium:

$$\partial_t^2\, \delta\rho = 4z\, (J(n+1)\ell)^2\, \nabla \left[\Delta_0^2\, \nabla \delta\rho \right], \qquad (4)$$

where $\Delta_0 = (1/2)\sin\theta$ is the local value of the order parameter vanishing at the boundaries of the Mott states. The form of Eq.(4) is identical to that governing a trapped Bose-Einstein condensate in the absence of a lattice [20] with Δ_0^2 playing the role of an equilibrium density of the condensate confined between two Mott states to an interlayer with radius r_n and width δr_n. It must be noted that while the equations governing density distortions are identical to those derived from the standard Gross-Pitaevskii formalism [20] for a condensate in the absence of a lattice, the equations of motion for the order parameter $\langle s^+ \rangle$ in general do not correspond to the Gross-Pitaevskii form, but reproduce it in the limit of small density distortions.

For the uniform case, the excitation spectrum can be obtained by treating the order parameter Δ_0 as spatially-independent. The eigenvalue equation, Eq. (4), is solved by the Fourier transformation, $\delta\rho \propto \exp(i\mathbf{pr} - i\omega_{\mathbf{p}} t)$, where $\mathbf{p}$ is the wave vector. The resulting sound mode,

$$\omega_{\mathbf{p}} = cp, \quad c = \sqrt{z} J(n+1)\ell |\sin\theta|, \qquad (5)$$

is related to the spontaneously-broken symmetry in the ordered state. According to the Landau criterion, the sound-like spectrum of Eq. (5) makes the ordered state a superfluid. One notices that the speed of sound, c, goes to zero as one approaches the Mott phases at $\sin\theta = 0$.

In the trapped geometry, an estimate of the excitation spectrum can be obtained from the quantization conditions imposed on the wave vector p in Eq.(5), with the speed of sound approximated by its value in the center of the layer, $c_0 = \sqrt{z} J(n+1)\ell$. For a spherically symmetric trap, the excitation modes are confined within an interlayer centered at radius r_n with width $\delta r_n = 2a_n$. The excitation modes terminate at the boundaries of the Mott regions, *i.e.* $p_j = j/a_n$ with $j = 0, 1, \ldots$, which gives a radial mode spectrum $\omega_j \simeq \Omega_r j$ with characteristic frequency $\Omega_r = J(n+1)\ell/a_n$. The quantization of the surface modes is related to the angular momentum $L = 0, 1, \ldots$ through $p_L = L/r_n$ which leads to the spectrum $\omega_L \simeq \Omega_a L$ with characteristic frequency $\Omega_a = \Omega_r a_n/r_n$. The degeneracy of the surface modes is $(2L+1)$ for each value of L. The perturbative calculation of the modes in Eq.(4) in the limit $a_n/r_n \ll 1$ confirms these estimates and gives the following result:

$$\left(\frac{\omega_{Lj}}{\Omega}\right)^2 \approx j(j+1) + \frac{a_n^2}{r_n^2}\left[1 + \frac{3}{(2j-1)(2j+3)}\right] + L(L+1)\frac{a_n^2}{2r_n^2}\left[1 - \frac{1}{(2j-1)(2j+3)}\right], \qquad (6)$$

where $\Omega = \sqrt{6}\,\Omega_r$, $j = 0, 1, \ldots$, $L = 0, 1, \ldots$, and $j + L \neq 0$. In the continuum approximation, the wavelength of the modes should be much larger than the lattice spacing, which sets upper bounds on the quantum numbers: $L \ll r_n/\ell$ and $j \ll a_n/\ell$. The second term in Eq.(6) is independent of L and is associated with the curvature of the interlayer; it vanishes at $j = 0$. The lowest energy modes for thin interlayers, $a_n/r_n \ll 1$, correspond to angular excitations ($j = 0$) given by $\omega_L = 2\Omega_a\sqrt{L(L+1)}$, $L = 1, 2, \ldots$.

We note that the mode spectrum of Eq. (6) corresponds to that of a condensate confined with an explicitly shell-shaped trap (for instance, a "bubble trap" in Ref. [21]) since the "effective confining potential" in Eq. (4) has the form $V_{eff} \propto (r - r_n)^2/a_n^2$ for thin interlayers. The calculation of the radial ($L = 0$) modes with $j = 1, 2$ in Ref. [22] confirms this connection for the lowest-lying radial modes (analogous to "breathers" in spherical condensates).

The characteristic frequencies Ω_r, Ω_a of the radial and angular modes set temperature scales at which the spectrum in Eq.(6) becomes quasiclassical, $j, L \gg 1$. For the aforementioned experimental parameters, the corresponding energy scales are of the order $\Omega_r \simeq 5\,\mathrm{nK}$, $\Omega_a \simeq 0.5\,\mathrm{nK}$. The energy of the system at finite temperature is obtained through quantization of the collective modes, $E(T) = \sum_{Lj}(2L+1)\omega_{Lj} n_{Lj}$, where $n_{Lj} = 1/(\exp(\omega_{Lj}/T) - 1)$ is the thermal occupation of the bosonic modes with spectrum given by Eq. (6), and the factor $(2L+1)$ takes into account the degeneracy of the angular modes. There are three temperature regimes in this case. In the extreme low-temperature limit, $T \ll \Omega_a$, thermal excitations are gapped, i.e. $E(T) \propto \Omega_a \exp(-2\sqrt{2}\Omega_a/T)$. At intermediate temperatures, $\Omega_a \ll T \ll \Omega_r$, the radial modes are frozen and only the two-dimensional angular modes contribute to the energy, $E(T) \propto T^3/\Omega_a^2$. At higher temperatures, $T \gg \Omega_r$, both radial and angular modes are excited, and the energy has a three-dimensional phonon-like temperature dependence, $E(T) \propto T^4/\Omega_r^3$. The separation of temperature scales achieved by changing the interlayer

width from $\delta r_n \simeq \ell$ to $\delta r_n \gg \ell$ tunes the effective dimensionality of the system from two to three dimensions.

At finite temperatures, the order parameter introduced in Eq.(3) is depleted from its zero temperature value by the collective modes. In the low-temperature regime, $T \ll J(n+1)$, for wide interlayers, $\delta r_n \gg \ell$, the order parameter depletion is similar to the case of a three-dimensional weakly-interacting BEC, $\delta\Delta(T) \propto (T/J(n+1))^2$. At higher temperatures, the long-range order is destroyed by the quasiparticle excitations whose wavelength is of the order of the lattice spacing. The critical temperature ought to be of the same order of magnitude as these excitations with the energies of order $J(n+1)$ (obtained from setting $j \simeq a_n/\ell$ and $L \simeq r_n/\ell$ in Eq.(6)). A mean-field calculation similar to the one in Ref.[17] confirms the estimate and provides a mean-field expression for the critical temperature $T_{3D} = 3J(n+1)$. Thermal properties of narrow interlayers, $\delta r_n \simeq \ell$, are qualitatively different. In this case the angular excitations play the dominant role. In accordance with the Mermin-Wagner-Hohenberg theorem [23], the long-range order is destroyed but the system retains power-law correlations in the phase of the order parameter. In the limit that the interlayer width is comparable to the lattice spacing, $\delta r_n \simeq \ell$, a simple model capturing the properties of the two-dimensional system involves only phase variables and leads to the effective Hamiltonian, $\mathcal{H}_\varphi = (K/2)\int d^2x\,(\nabla\varphi)^2$, where the integration is over the surface of the spherical layer, and we have introduced the phase stiffness $K = J(n+1)/2$. The Kosterlitz-Thouless (K-T) transition [24] between the high-temperature normal and the low-temperature superfluid state occurs at temperature $T_{2D} = (\pi/2)K = (\pi/4)J(n+1)$. At intermediate widths, $\delta r_n \gtrsim \ell$, the phase stiffness is approximated by $K = (J(n+1)/2)(\delta r_n/\ell)\overline{\sin^2\theta}$ with $\overline{\sin^2\theta} = (1/\delta r_n)\int dr \sin^2\theta$. For the interlayer in the trap $\overline{\sin^2\theta} = 2/3$, and the critical temperature of the K-T transition is given by $T_c = (\pi/6)(\delta r_n/\ell)J(n+1)$, which is a linear function of the interlayer width, interpolating between two-dimensional and three-dimensional limits, $T_{2D} \leq T_c \leq T_{3D}$. In the range of current experiments, for $J \approx h \times 120$Hz, one obtains an estimate of the critical temperature, $T_c \simeq 10\,$nK.

In conclusion, we have shown that the interlayer with fluctuating site occupation confined between two Mott states becomes superfluid at low but experimentally accessible temperatures. Employing the pseudospin model, we have identified the effective potential confining the superfluid and analyzed the low-energy excitations in the system. We have demonstrated that the effective dimensionality of the interlayer can be changed by tuning external parameters. As an example of the ensuing physics we have suggested that the critical temperature interpolates between two-dimensional and three-dimensional limits as one changes the width of the interlayer. A clear experimental signature of the interlayer condensate, either through time-of-flight and interference experiments, excitation of collective modes or radio-frequency spectroscopy is yet to be obtained.

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